

Energy Diffusion and Heat Conduction Near Thermal Equilibrium

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(Dated: revised on 9 Mar 2012)

We derive *analytically* a dynamical equality relating the mean square displacement of energy diffusion near equilibrium to the autocorrelation function of total heat flux fluctuation in equilibrium. This relation is a direct consequence of the microscopic energy conservation law. We numerically verify the dynamical equality for typical nonlinear lattice systems, and also show some special consequences of this dynamical equality, in particular, the connection between anomalous heat conduction and anomalous energy diffusion without *a priori* assumption for the underlying diffusion processes.

PACS numbers: 05.60.-k, 05.20.-y, 44.10.+i, 66.70.-f

It is well known that normal heat conduction is related to normal diffusion. For example, in a 1D continuous system, the Fourier's law of heat conduction states that $j(x, t) = -\kappa \partial_x T(x, t)$, where $j(x, t)$ is the local heat flux density, $T(x, t)$ the local temperature and κ the thermal conductivity. From energy continuity equation $\partial_t \varepsilon(x, t) + \partial_x j(x, t) = 0$, one obtains $\partial_t \varepsilon(x, t) = \kappa \partial_x^2 T(x, t)$. Assuming local thermal equilibrium exists and temperature change is small, the local energy density can be simply related to the local temperature as $\varepsilon(x, t) = c_V T(x, t)$, where c_V is the specific heat. Therefore, one reaches the familiar heat equation describing normal diffusion $\partial_t T(x, t) = D \partial_x^2 T(x, t)$, where the diffusion constant D is linked with heat conductivity κ through $D = \kappa / c_V$ [1].

The discovery of anomalous heat conduction [2] in 1D Fermi-Pasta-Ulam (FPU) and FPU-like lattices has attracted enormous theoretical [3–6] and experimental [7, 8] studies of the length-dependent heat conductivity in low dimensional systems. In such systems, the asymptotic heat conductivity can be expressed as

$$\kappa \propto L^\alpha. \quad (1)$$

On the other hand, for the diffusion processes of particles [9], which could be heat carriers, it is established that the mean square displacement (MSD) of particles increases with time as

$$\overline{x^2}(t) \propto t^\gamma. \quad (2)$$

Since the Fourier's law ($\alpha = 0$) can be connected to normal diffusion ($\gamma = 1$), it is commonly believed that anomalous heat conduction ($\alpha \neq 0$) should somehow be related to anomalous diffusion ($\gamma \neq 1$). The pioneering works in this direction have given rise to insightful albeit controversial analytical results [10, 11] for billiard models. Further numerical investigations of energy diffusion in 1D lattice systems [12–15] confirmed the relation $\alpha = \gamma - 1$ between heat conduction and diffusion as predicted by Ref. [11]. However, the analytical derivation of this relation is only available for the simple

non-interacting billiard model under a strong assumption that the moving particles obey a pre-defined Lévy walk distribution. Therefore, this result is still restricted to dealing with the particle diffusion cases. Actually, similar relation between electric conduction and diffusion has also been investigated in the context of the diffusion of charged particles [16].

However, energy transport in discrete lattices is a completely different phenomenon. The heat carriers are phonons which are defined in momentum space and do not move in the real space [17]. Therefore the definition of “displacement” of energy is not clear. We do not have the quantity “mean square displacement” of energy using which we are able to characterize energy diffusion in these lattice cases. As a consequence, the previous inspiring works that tried to bridge energy diffusion and heat conduction from the aspect of particle diffusion have only limited application. A fundamental theory for lattice models in this area is still lacking, although some heuristic results are available [13, 15].

Therefore, to build a general and rigorous theory connecting energy diffusion and heat conduction that does not rely on any *a priori* assumption on the details of the system and can be applied to any model as well as lattices is still challenging and remains to be one of the most outstanding problems in statistical physics.

In this Letter, based on a rigorous linear response description of energy diffusion, we derive *analytically* a dynamical equality connecting the MSD of the nonequilibrium energy diffusion $\overline{x^2}(t)$ and the autocorrelation function of total heat flux, $C(t)$, in equilibrium:

$$\frac{d^2}{dt^2} \overline{x^2}(t) = \frac{2C(t)}{k_B T^2 c_V}, \quad (3)$$

where c_V is the heat capacity per unit length, k_B the Boltzmann constant, and T the temperature. Our derivation does not rely on any special details of the model or any assumption about the diffusion process. It is a direct consequence of microscopic energy conservation. In this sense, the equality we derived is a fundamental and intrinsic relation between energy diffusion and heat conduction. We further numeri-

cally verify our dynamical equality by using two paradigmatic 1D nonlinear lattice systems, *i.e.*, ϕ^4 lattice showing normal heat conduction and quartic FPU- β (qFPU- β) lattice exhibiting anomalous heat conduction.

Derivation For simplicity, we limit ourselves to a 1D continuous system. The generalization of the derivation to higher dimensional and discrete lattice cases is straightforward. In thermal equilibrium, we have the microscopic energy continuity equation:

$$\partial_t \epsilon(x, t) + \partial_x j(x, t) = 0. \quad (4)$$

where $j(x, t)$ denotes the local heat flux density at position x at time t . We have used the energy density fluctuation $\epsilon(x, t) = \Delta \epsilon(x, t) \equiv \epsilon(x, t) - \langle \epsilon(x, t) \rangle$ to replace the energy density $\epsilon(x, t)$ in the above equation because the difference between them is a time-independent constant. $\langle \cdot \rangle$ denotes the canonical ensemble average.

The continuity equation (4) connects local energy density fluctuation with local heat flux density. To find the further connection between correlation functions of these two quantities, we multiply Eq. (4) by $\epsilon(x', t')$ and $j(x', t')$ respectively, and take the ensemble average:

$$\partial_t \langle \epsilon(x, t) \epsilon(x', t') \rangle + \partial_x \langle j(x, t) \epsilon(x', t') \rangle = 0, \quad (5)$$

$$\partial_t \langle \epsilon(x, t) j(x', t') \rangle + \partial_x \langle j(x, t) j(x', t') \rangle = 0. \quad (6)$$

For a homogeneous system in thermal equilibrium, the correlation functions $\langle \epsilon(x, t) \epsilon(x', t') \rangle$, $\langle j(x, t) \epsilon(x', t') \rangle$, $\langle \epsilon(x, t) j(x', t') \rangle$ and $\langle j(x, t) j(x', t') \rangle$ only depend on spatial separation and time differences. Therefore we can define $\mathcal{C}_{AB}(x - x', t - t') = \mathcal{C}_{BA}(x' - x, t' - t) \equiv \langle A(x, t) B(x', t') \rangle$, where A, B takes the form of ϵ, j . It is then easy to verify that the cross correlation terms $\mathcal{C}_{j\epsilon}(x, t)$ and $\mathcal{C}_{\epsilon j}(x, t)$ are invariant under the transformation of $(x, t) \rightarrow (-x, -t)$. Therefore, we have $\mathcal{C}_{j\epsilon}(x - x', t - t') = \mathcal{C}_{\epsilon j}(x - x', t - t')$. By performing ∂_t to Eq. (5) and ∂_x to Eq. (6), and subtracting the cross terms, we obtain:

$$\partial_t^2 \mathcal{C}_{\epsilon\epsilon}(x, t) = \partial_x^2 \mathcal{C}_{jj}(x, t). \quad (7)$$

As we shall see soon, the r.h.s. of Eq. (7) is actually connected to the equilibrium autocorrelation of total heat flux $C(t)$ and the l.h.s. is closely connected to the MSD $\overline{x^2}(t)$ of the nonequilibrium energy diffusion.

The autocorrelation function of total heat flux is defined as

$$C(t) = \lim_{L \rightarrow \infty} \frac{1}{L} \langle J_L(t) J_L(0) \rangle, \quad (8)$$

where $J_L = \int_{-L/2}^{L/2} j(x, t) dx$ is the total heat flux for 1D system with length L . Thus $C(t)$ can be expressed as

$$\begin{aligned} C(t) &= \lim_{L \rightarrow \infty} \frac{1}{L} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \mathcal{C}_{jj}(x - x', t) dx dx' \\ &= \int \mathcal{C}_{jj}(x, t) dx, \end{aligned} \quad (9)$$

where \int is short for $\int_{-\infty}^{\infty}$ throughout the paper. Now, the connection between the r.h.s of Eq. (7) and $C(t)$ has been established.

Before we come to the connection between the l.h.s of Eq. (7) and the MSD $\overline{x^2}(t)$, we need to obtain the energy distribution $\rho(x, t)$ describing nonequilibrium energy diffusion so that the MSD, or the variance of the energy distribution, can be defined as

$$\overline{x^2}(t) = \int x^2 \rho(x, t) dx. \quad (10)$$

It should be stressed that the MSD $\overline{x^2}(t)$ is not measured in the canonical ensemble as denoted by $\langle \cdot \rangle$. Instead, it is defined in a non-stationary irreversible diffusion process described by the probability distribution of energy $\rho(x, t)$.

The scenario of energy diffusion is given as follows: firstly, an energy perturbation is imposed on the initially equilibrated system at temperature T . Then after removing the perturbation, the energy diffusion process is just the relaxation of the energy excitation. Following Ref. [4], the external perturbative Hamiltonian is introduced as

$$H_{ext}(t) = -\theta(-t) \int dx \epsilon(x, t) \frac{\Delta T(x)}{T}, \quad (11)$$

under the assumption of local thermal equilibrium, where $\theta(t)$ is the Heaviside function which indicates the perturbation is removed at time $t = 0$ after it has been applied from the infinite past. As we will see soon, $\Delta T(x)$ describes the energy profile before relaxation. The form of $\Delta T(x)$ will not affect our main result, namely, Eq. (3) is generic and does not depend on the specific initial energy profile.

Provided $|\Delta T(x)|$ is sufficiently small, we can apply the linear response theory [18] to study the energy distribution during the diffusion process such that for $t \geq 0$ the response of $\epsilon(x, t)$ to the perturbation is

$$\begin{aligned} \delta \epsilon(x, t) &= \int_{-\infty}^t \theta(-t') dt' \int dx' \Phi_{\epsilon\epsilon}(x - x', t - t') \frac{\Delta T(x')}{T} \\ &= \frac{1}{T} \int_t^{\infty} dt' \int dx' \Phi_{\epsilon\epsilon}(x - x', t') \Delta T(x'). \end{aligned} \quad (12)$$

$\Phi_{\epsilon\epsilon}(x, t)$ is known as the response function which relates to the *equilibrium* correlation of energy fluctuation as [18] $\Phi_{\epsilon\epsilon}(x, t) = -\beta_T \langle \epsilon(0, 0) \dot{\epsilon}(x, t) \rangle = -\beta_T \dot{\mathcal{C}}_{\epsilon\epsilon}(x, t)$, where $\dot{\cdot}$ denotes time derivative and $\beta_T = (k_B T)^{-1}$. Using the condition $\mathcal{C}_{\epsilon\epsilon}(x, \infty) = 0$, we obtain

$$\delta \epsilon(x, t) = \int dx' \mathcal{C}_{\epsilon\epsilon}(x - x', t) \frac{\Delta T(x')}{k_B T^2}, \quad (13)$$

which describes the evolution of energy profile in the diffusion process.

At time $t = 0$, the total energy excited in the system $\delta \bar{E} = \int \delta \epsilon(x, 0) dx$ reads

$$\delta \bar{E} = \iint dx dx' \mathcal{C}_{\epsilon\epsilon}(x - x', 0) \frac{\Delta T(x')}{k_B T^2} = \int c_V \Delta T(x') dx', \quad (14)$$

where $\int \mathcal{C}_{ee}(x, 0)dx = k_B T^2 c_V$ is used [19]. This result implies an expected result that the total energy excited is the accumulation of local energy perturbation. Actually, when the interaction in the system is short ranged, the simultaneous correlation of energy density can be approximated as $\mathcal{C}_{ee}(x, 0) \sim \delta(x)$, then the energy profile at $t = 0$ can be simplified as $\delta\bar{\varepsilon}(x, 0) = c_V \Delta T(x)$. In this aspect, $\Delta T(x)$ describes the initial excitation profile of energy diffusion.

In view of the analysis above, the normalized energy distribution in the diffusion process is written as

$$\rho(x, t) = \frac{\delta\bar{\varepsilon}(x, t)}{\delta\bar{E}} = \frac{1}{\mathcal{N}} \int dx' \mathcal{C}_{ee}(x - x', t) \Delta T(x'), \quad (15)$$

where $\mathcal{N} = k_B T^2 c_V \int \Delta T(x') dx'$ is the normalization constant. From energy conservation, it is expected that $A(t) = \int \rho(x, t) dx$ should always be unity. Using Eq. (7), this can be proved as follows. Since $d^2 A(t)/dt^2 = \iint \partial_x^2 \mathcal{C}_{jj}(x - x', t) \Delta T(x') dx dx' / \mathcal{N} \equiv 0$, together with $dA(0)/dt = 0$ from the even parity of $\mathcal{C}_{ee}(x, t)$ with respect to t and $A(0) = 1$ by the definition of $\rho(x, t)$, we get $dA(t)/dt = 0$ and $A(t) = 1$.

For a special perturbation $\Delta T(x) \propto \delta(x)$, Eq. (15) reduces to $\rho(x, t) = \mathcal{C}_{ee}(x, t)/k_B T^2 c_V$. This result is reminiscent of a heuristic definition for discrete lattices $\rho(i, t) = \langle \Delta H_0(0) \Delta H_i(t) \rangle / \langle \Delta H_0(0) \Delta H_0(0) \rangle$ [13] provided $\langle \Delta H_0(0) \Delta H_0(0) \rangle = k_B T^2 c_V$, where $H_i(t)$ is the local energy of site i in the lattice, the discrete analogue of $\varepsilon(x, t)$. However, this condition implies $\langle \Delta H_0(0) \Delta H_i(0) \rangle = 0$ for $i \neq 0$ or its continuous version $\mathcal{C}_{ee}(x, 0) = k_B T^2 c_V \delta(x)$, which has more restrictions on the system, *e.g.*, short ranged interaction and special definition for the local energy [21]. Therefore, our result Eq. (15) is more general and rigorous.

To describe the evolution of the MSD, from Eq. (7), (10) and (15), we obtain

$$\frac{d^2 \bar{x}^2(t)}{dt^2} = \frac{1}{\mathcal{N}} \iint x^2 \partial_x^2 \mathcal{C}_{jj}(x - x', t) \Delta T(x') dx dx'. \quad (16)$$

Because $\int \mathcal{C}_{jj}(x, t) dx$ exists as indicated in Eq. (9), we have the boundary conditions $\lim_{x \rightarrow \infty} x^2 \partial_x \mathcal{C}_{jj}(x, t) = 0$ and $\lim_{x \rightarrow \infty} x \mathcal{C}_{jj}(x, t) = 0$. By performing integration by parts twice on Eq. (16) with respect to x , we finally arrive at our central result Eq. (3) for arbitrary $\Delta T(x)$.

This dynamical equality is essentially the equation of motion for the MSD of energy diffusion. Its initial conditions are specified as $\bar{x}^2(0) = \iint x^2 \mathcal{C}_{ee}(x - x', 0) \Delta T(x') dx dx' / \mathcal{N}$ and $d\bar{x}^2(0)/dt = 0$. The first one reduces to $\bar{x}^2(0) = 0$ if $\mathcal{C}_{ee}(x, 0)$ and $\Delta T(x)$ are both δ -functions. The second one results from the even parity of $\mathcal{C}_{ee}(x, t)$ with respect to t provided it exists [22]. These initial conditions imply that the lowest two terms of Taylor series of $\bar{x}^2(t)$ at $t = 0$ should be $a_0 + a_2 t^2$, with $a_0 = \bar{x}^2(0)$ and $a_2 = C(0)/k_B T^2 c_V$. Therefore, realistic energy diffusion process should start as a ballistic transport. Similar phenomenon for particle diffusion has already been observed in experiments recently [23].

As the central result of our work, Eq. (3) relates the MSD $\bar{x}^2(t)$ of the nonequilibrium energy diffusion and the equilibrium autocorrelation function of total heat flux, $C(t)$. This relation bridges the heat conduction and energy diffusion in the sense that: (1) heat conduction is related to the autocorrelation function $C(t)$ [24]; (2) energy diffusion processes can be classified through the distinct behaviors of MSD $\bar{x}^2(t)$ [9].

We should stress that Eq. (3) is derived without any explicit *prior* assumption on the details of the system and diffusion process. The derivation is independent of the initial condition of energy diffusion. It is an intrinsic relation purely coming from the microscopic energy conservation law.

Simulation In order to verify Eq (3), we perform equilibrium numerical simulations on 1D nonlinear lattices with a general dimensionless Hamiltonian:

$$H = \sum_i H_i; \quad H_i = \frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_i), \quad (17)$$

where q_i and p_i denotes the displacement and momentum, $V(q)$ the inter-particle potential, $U(q)$ the on-site potential and H_i the local Hamiltonian or energy. We adopt the definition in Ref. [4] for the local heat flux $j_i(t) = -\dot{q}_i \partial V(q_i - q_{i-1}) / \partial q_i$ and the total heat flux $J(t) = \sum_i j_i(t)$. The energy distribution is calculated according to the discrete form of Eq. (15), *i.e.*, $\rho(i, t) = \langle \Delta H_0(0) \Delta H_i(t) \rangle / k_B T^2 c_V$ with $\Delta H_i(t) \equiv H_i(t) - \langle H_i(t) \rangle$. The MSD is calculated as $\bar{x}^2(t) = \sum_i i^2 \rho(i, t)$. The Boltzmann constant k_B is set as unit. We note that different definitions of local energy and heat flux do not affect the verification as long as they are defined consistently according to energy conservation law. The Hamiltonian is integrated using the fourth order symplectic scheme *cSABA*₂ [25, 26] with

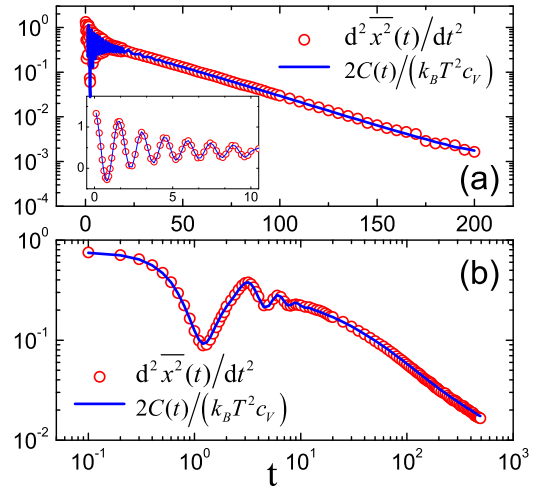


FIG. 1: Numerical verification of Eq. (3) for (a) the diffusive ϕ^4 lattice ($N = 501$, $T = 0.441$, $c_V = 0.885$ [21]); and (b) the superdiffusive qFPU- β lattice ($N = 601$, $T = 0.020$, $c_V = 0.750$). $h = 0.1$ is used for small t while $h = 5$ (qFPU- β) or 10 (ϕ^4) for large t in order to reduce the fluctuation.

time step $\Delta t = 0.05$ which usually conserves the total energy with a relative deviation of the order of 10^{-6} after a total time 10^7 . The second derivative of the MSD is calculated as $d^2\overline{x^2}(t)/dt^2 = [\overline{x^2}(t+h) - 2\overline{x^2}(t) + \overline{x^2}(t-h)]/h^2$ where h is the time interval.

Our numerical verification is performed on the ϕ^4 lattice with $V(q) = q^2/2$, $U(q) = q^4/4$ and the q FPU- β lattice with $V(q) = q^4/4$, $U(q) = 0$, respectively. The former is a paradigmatic lattice system showing *normal* heat conduction [27, 28]. The latter is just the high temperature limit of the FPU- β model, a well studied lattice system exhibiting *anomalous* heat conduction [29–32]. The q FPU- β lattice has temperature independent heat capacity $c_V = 3/4$ which can be easily deduced from the generalized equipartition theorem $\langle z\partial_z H \rangle = k_B T$ for any canonical coordinate $z = q_i, p_i$; while the heat capacity for ϕ^4 lattice is temperature dependent which is calculated from $c_V(T) = \partial_T \langle E(T) \rangle / N$, where $E(T)$ is the total energy of the system at temperature T [21]. The numerical results in Fig. (1) show perfect agreement with the dynamical equality (3) for both models, which demonstrate its universality.

Application In the following, we will show some special corollaries of Eq. (3), with only the help of Green-Kubo (GK) formula [24].

(1): If the energy diffusion is *normal*, we have $\lim_{t \rightarrow \infty} \overline{x^2}(t)/2t = D$, where D is a finite constant called thermal diffusivity. From the GK formula and noticing the initial conditions for $\overline{x^2}(t)$, we obtain the thermal conductivity:

$$\kappa^{\text{normal}} = \int_0^\infty \frac{C(t)}{k_B T^2} dt = \frac{c_V}{2} \lim_{t \rightarrow \infty} \frac{d\overline{x^2}(t)}{dt} = c_V D. \quad (18)$$

We shall emphasize that although Eq. (18) is well accepted, it was obtained by the aids of a presumed empirical Fourier's law, or equivalently the heat equation, as shown at the beginning of this paper. However, we have demonstrated here that it is a rigorous result from Eq. (3) and does not rely on the Fourier's law any more.

Particularly, if we assume an exponential relaxation of the flux autocorrelation function $C(t) = C_0 e^{-t/\tau}$ similar to the ϕ^4 lattice in Fig. (1a), with τ the characteristic relaxation time, the MSD can be obtained by integrating Eq. (3) twice, reading

$$\overline{x^2}(t) = 2D \left[t - \tau \left(1 - e^{-\frac{t}{\tau}} \right) \right]. \quad (19)$$

The asymptotic behavior is $\overline{x^2}(t) \sim 2Dt$ with diffusivity $D = C_0 \tau / (k_B T^2 c_V)$. The thermal conductivity is $\kappa = \int_0^\infty C(t) dt / (k_B T^2) = C_0 \tau / (k_B T^2)$, so that κ and D satisfy the corollary Eq. (18). We also notice that in the short time limit $t \ll \tau$, Eq. (19) implies ballistic transport $\overline{x^2}(t) = v^2 t^2$, where $v = \sqrt{C_0 / (k_B T^2 c_V)}$ can be regarded as the speed of the collective energy propagation in the ballistic limit. The heat conductivity can be expressed as $\kappa = c_V v^2 \tau$ which is reminiscent of the kinetic theory. It can be noticed that $\overline{x^2}(t)$

in Eq. (19) has exactly the same time dependence as the MSD of Brownian motion described by the Langevin equation [18].

(2): If the energy diffusion is *superdiffusive*, then asymptotically we have $\overline{x^2}(t) \sim t^\gamma$ with $1 < \gamma < 2$. From the equality Eq. (3) we get $C(t) \sim t^\delta$ with $\delta = \gamma - 2$. The GK formula is not applicable due to the divergence of $\int_0^\infty C(t) dt$. Thus we get anomalous heat conduction with infinite conductivity in the thermodynamic limit. However, if one is interested in a length-dependent heat conductivity, one can follow the heat conduction review literatures [4, 5] to put a cut-off time to the GK formula. Although not rigorously proved, it is commonly reasoned as that for a finite system, sound waves travels to the boundaries at a constant speed c_s , which will lead to a fast decay of correlations at time $t \sim L/c_s$ [5]. In this case, our central result Eq. (3) gives

$$\kappa_L^{\text{super}} \sim \frac{1}{k_B T^2} \int_0^{L/c_s} C(t) dt = \frac{c_V}{2} \frac{d\overline{x^2}(t)}{dt} \Big|_{t \sim L/c_s}, \quad (20)$$

which leads to the asymptotic behavior of the length-dependent thermal conductivity $\kappa_L^{\text{super}} \sim L^\alpha$ with

$$\alpha = \delta + 1 = \gamma - 1. \quad (21)$$

This reproduces the relation $\alpha = \gamma - 1$ derived for a billiard model with the particles follow the *a priori* Lévy walk process [11]. On the contrary, our derivation is a direct consequence of the microscopic energy conservation law and does not rely on any assumption on the specific models and the diffusion processes. It is fulfilled in the whole time range of the diffusion process. In this sense, our dynamical equation (3) is intrinsic and more fundamental than a simple relation between γ and α .

(3): Let us look into a situation in which the MSD $\overline{x^2}(t)$, based on the equilibrium energy spatiotemporal correlation Eq. (15), has the asymptotic form $\overline{x^2}(t) \sim t^\gamma$ with $0 < \gamma < 1$, which corresponds to the *subdiffusive* case. From Eq. (3), we get $C(t) \sim \gamma(\gamma - 1)t^{\gamma-2}$. The exponent $\delta = \gamma - 2 < -1$ so that $C(t)$ is integrable over $[0, \infty)$ and the GK formula is still applicable. From Eq. (3), we have

$$\kappa^{\text{sub}} = \lim_{t \rightarrow \infty} \frac{c_V}{2} \frac{d\overline{x^2}(t)}{dt} \sim \lim_{t \rightarrow \infty} t^{\gamma-1} = 0. \quad (22)$$

This is an expected result which indicates a subdiffusive system is a perfect thermal insulator in the thermodynamic limit. If we again adopt the “cut-off-time” reasoning for finite system, Eq. (20) and (21) will still be valid and the heat conductivity will decay as, $\kappa_L^{\text{sub}} \sim L^{\gamma-1}$, asymptotically.

It is interesting to note that when t is large, the autocorrelation function $C(t)$ should be negative since its coefficient $\sim \gamma(\gamma - 1) < 0$. This is in stark contrast to the case where $C(t) \sim t^\delta$ with $\delta < -1$ but has a positive coefficient, which will result in a finite conductivity and thus implies normal diffusion [4, 33].

In conclusion, we have *analytically* derived an exact *dynamical* equality, Eq. (3), for all isotropic systems which

bridges energy diffusion and heat conduction in terms of the MSD of the nonequilibrium energy diffusion, $\overline{x^2}(t)$, and the equilibrium autocorrelation function of total heat flux, $C(t)$.

This relation is a natural consequence of microscopic energy conservation law and is thus *intrinsic* and more fundamental than the previously derived relation $\alpha = \gamma - 1$. In principle, it can be applied to isotropic systems in any dimension

From this equality, we are able to recover the theories for normal and anomalous heat conduction. The validity of this intrinsic relation has been verified with two paradigmatic 1D nonlinear lattice systems, *i.e.*, the ϕ^4 lattice which shows normal heat conduction and the q FPU- β lattice which exhibits anomalous heat conduction. The perfect agreements between theory and numerical simulations demonstrate its universality.

At last, we would like to mention that the present results are derived in the linear response framework. Whether there exist universal relations beyond linear response regime to unify heat conduction and energy diffusion is still an open question and requires further investigation.

We would like to thank Lifa Zhang, Jie Chen, Guimei Zhu and Lina Yang in NUS and Sergej Flach, Victor Fleurov, Petrutza Anghel-Vasilescu in MPIPKS for useful discussions. Special thanks to Joshua D. Bodyfelt for the help of distributed computation in cluster. This work was supported in part by a grant W-144-000-280-305 from SERC of A*STAR, Singapore, and by a grant W-144-000-285-646 from National University of Singapore, and the start-up fund (NL and BL) from Tongji University.

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- [22] For an example that $dx^2(0)/dt$ does not exist, consider ideal normal diffusion described by heat equation which satisfies $\overline{x^2}(t) \equiv 2D|t|$. So $d\overline{x^2}(t)/dt$ at time $t = 0$ is ill-defined. Actually, in this case, we can get $C(t) = 2k_B T^2 c_V D \delta(t)$ from Eq. (3). It is an unrealistic process. For an example of normal diffusion that is more realistic, please refer to the *Application* part.
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